FTMW STUDY OF THE CHIRALITY RECOGNITION BETWEEN TWO DIFFERENT CHIRAL MOLECULES: THE GLYCIDOL-PROPYLENE OXIDE COMPLEX

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The chirality recognition effect between the prototype chiral molecular systems, i.e. glycidol and propylene oxide has been studied using rotational spectroscopy and high level ab initio calculations. Extensive ab initio calculations have been performed to locate all possible low energy conformers of the diastereomeric pair and *twenty eight* minima have been found. The four most sable hetero and four homo chiral dimers, formed from the two lowest energy monomer conformations G+g- and G-g+ of the glycidol, were predicted to be close in their stability. Jet-cooled rotational spectra of some of them have been detected using a pulsed molecular beam Fourier transform microwave spectrometer and been assigned for the first time. All the low energy binary conformers observed show one primary intermolecular OH- - -O hydrogen bond and two secondary intermolecular CH- - -O hydrogen bonds. The induced fit phenomenon detectedwill be discussed.